

Tetraphenylmethane

Other names:	Benzene, 1,1',1'',1'''-methanetetrayltetrakis-Methane, tetraphenyl-
Inchi:	InChI=1S/C25H20/c1-5-13-21(14-6-1)25(22-15-7-2-8-16-22,23-17-9-3-10-18-23)24-19-1
InchiKey:	PEQHIRFAKIASBK-UHFFFAOYSA-N
Formula:	C25H20
SMILES:	<chem>c1ccc(C(c2ccccc2)(c2ccccc2)c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	320.43
CAS:	630-76-2

Physical Properties

Property code	Value	Unit	Source
chs	-12988.00	kJ/mol	NIST Webbook
chs	-13000.00	kJ/mol	NIST Webbook
chs	-12943.20 ± 2.50	kJ/mol	NIST Webbook
gf	612.10	kJ/mol	Joback Method
hf	398.10 ± 6.90	kJ/mol	NIST Webbook
hf	393.00 ± 6.30	kJ/mol	NIST Webbook
hfs	247.20 ± 4.10	kJ/mol	NIST Webbook
hfs	292.00	kJ/mol	NIST Webbook
hfus	29.26	kJ/mol	Joback Method
hsub	151.00 ± 4.20	kJ/mol	NIST Webbook
hsub	140.00 ± 1.30	kJ/mol	NIST Webbook
hsub	151.00 ± 4.00	kJ/mol	NIST Webbook
hsub	150.90 ± 5.60	kJ/mol	NIST Webbook
hvap	79.05	kJ/mol	Joback Method
ie	8.41	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-7.80		Aqueous Solubility Prediction Method
logp	6.069		Crippen Method
mvol	268.070	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
sg	639.00	J/mol×K	NIST Webbook
tb	874.89	K	Joback Method
tc	1163.44	K	Joback Method
tf	556.15 ± 1.50	K	NIST Webbook
tf	554.60 ± 1.00	K	NIST Webbook

tf	555.65	K	Aqueous Solubility Prediction Method
tf	553.15 ± 3.00	K	NIST Webbook
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.89	J/mol×K	1115.35	Joback Method
cpg	855.92	J/mol×K	1067.26	Joback Method
cpg	842.21	J/mol×K	1019.17	Joback Method
cpg	827.45	J/mol×K	971.07	Joback Method
cpg	811.35	J/mol×K	922.98	Joback Method
cpg	793.59	J/mol×K	874.89	Joback Method
cpg	881.43	J/mol×K	1163.44	Joback Method
cps	368.20	J/mol×K	298.50	NIST Webbook
dvisc	0.0007604	Paxs	479.61	Joback Method
dvisc	0.0000434	Paxs	874.89	Joback Method
dvisc	0.0000576	Paxs	809.01	Joback Method
dvisc	0.0000804	Paxs	743.13	Joback Method
dvisc	0.0001197	Paxs	677.25	Joback Method
dvisc	0.0001941	Paxs	611.37	Joback Method
dvisc	0.0003538	Paxs	545.49	Joback Method
hfust	48.28	kJ/mol	554.20	NIST Webbook
hsubt	135.40 ± 1.30	kJ/mol	373.00	NIST Webbook
hsubt	143.30	kJ/mol	435.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C630762&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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